Electronic supplementary information

Theoretical insights into the structural, relative stable, electronic, and gas sensing properties of Pb_nAu_n (n=2-12) clusters: a DFT study

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Table S1 Calculated bond distances R (Å), vibrational frequencies υ (cm^{-1}), and vertical ionization potential energies VIPs (eV) of Au_2 dimer and Pb_2 dimer at different levels, and that of experimental data for Au_2 dimer and Pb_2 dimer.

System	Functional	Property	This work	Experiment
Au_2 dimer	GGA/PW91	R	2.49	2.47 [1]
	GGA/BPE		2.49	
	GGA/BLYP		2.53	
	GGA/PW91	υ	183.44	190.9 [1]
	GGA/BPE		181.92	
	GGA/BLYP		169.57	
	GGA/PW91	VIP	9.37	9.5 [2]
	GGA/BPE		9.30	
	GGA/BLYP		9.19	
Pb_2 dimer	GGA/PW91	R	2.95	2.93 [3]
	GGA/BPE		2.96	
	GGA/BLYP		2.99	
	GGA/PW91	υ	122.99	110 [3]
	GGA/BPE		120.05	
	GGA/BLYP		117.76	
	GGA/PW91	VIP	6.55	6.2 [4]
	GGA/BPE		6.56	
	GGA/BLYP		6.41	
PbAu cluster	GGA/PW91	R	2.67	
	GGA/BPE		2.67	
	GGA/BLYP		2.71	
	GGA/PW91	υ	149.10	
	GGA/BPE		148.99	
	GGA/BLYP		138.52	
	GGA/PW91	VIP	6.88	
	GGA/BPE		6.81	

	GGA/BLYP		6.83	

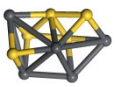
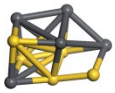
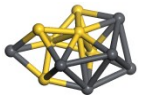
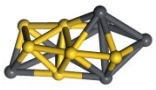
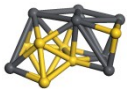
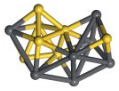
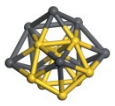
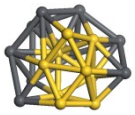
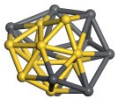
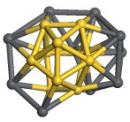
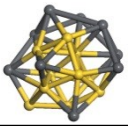
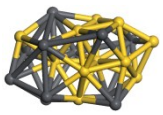
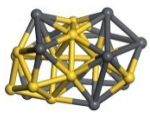
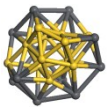
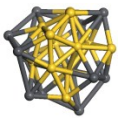
					
2a, ΔE=0 eV	2b, ΔE=0.0001 eV	3a, ΔE=0 eV	3b, ΔE=0.0006 eV	4a, ΔE=0 eV	4b, ΔE=0.1175 eV
					
5a, ΔE=0 eV	5b, ΔE=0,0001 eV	6a, ΔE=0 eV	6b, ΔE=0.2106 eV	7a, ΔE=0 eV	7b, ΔE=0.0016 eV
					
8a, ΔE=0 eV	8b, ΔE=0.5032 eV	9a, ΔE=0 eV	9b, ΔE=0.0231 eV	10a, ΔE=0 eV	10b, ΔE=0.1173eV
					
11a, ΔE=0 eV	11b, ΔE=0.0973 eV	12a, ΔE=0 eV	12b, ΔE=0.0286 eV		

Figure S1 Low energy structures of Pb_nAu_n (n=2-12) clusters. Configuration a represents the lowest energy structure, and configuration b stand for the second lowest energy structure of the the corresponding Pb_nAu_n (n=2-12) clusters. The energy differences represent the energy differences between the lowest energy structures and the second lowest energy structures. The dark grey ball is Pb atom, and yellow ball is Au atom.

References

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